Fourier Transform Infrared Spectroscopy

C.C. Homes
Department of Physics
Brookhaven National Laboratory

July 19, 2001

1 Fourier Transform Spectroscopy

Since its inception, most interferometer designs have incorporated some element of a basic Michelson interferometer, shown schematically in Figure 1. Both beams have been transmitted once and reflected once as they are divided at the beamsplitter, then reflected at either the movable (M1) or fixed (M2) mirror, and finally recombined at the beam splitter to proceed to the sample area and the detector.

Consider an incoming monochromatic plane wave with an average electric field amplitude E_m, frequency ω and wave number $\bar{\nu}$ (which as units of cm^{-1}):

$$\bar{\nu} = \frac{1}{\lambda} = \frac{\omega}{2\pi c} \tag{1}$$

(where λ is in cm), incident on the beam splitter (where c is the speed of light)

$$\vec{E} = \vec{E}_m \cos(\omega t - 2\pi\bar{\nu}y). \tag{2}$$

The beam from the mirror M2 after leaving the beam splitter in the direction of the condensing unit may be written as

$$\vec{E}_2 = rtc\vec{E}_m \cos\left[\omega t - 2\pi\bar{\nu}y_1\right] \tag{3}$$

where r is the reflectance (amplitude) of the beam splitter, t is the transmittance, and c is a constant depending on the polarization. Similarly from the other mirror M1, at the same point then we have

$$\vec{E}_2 = rtc\vec{E}_m \cos\left[\omega t - 2\pi\bar{\nu}(y_1 + x)\right] \tag{4}$$

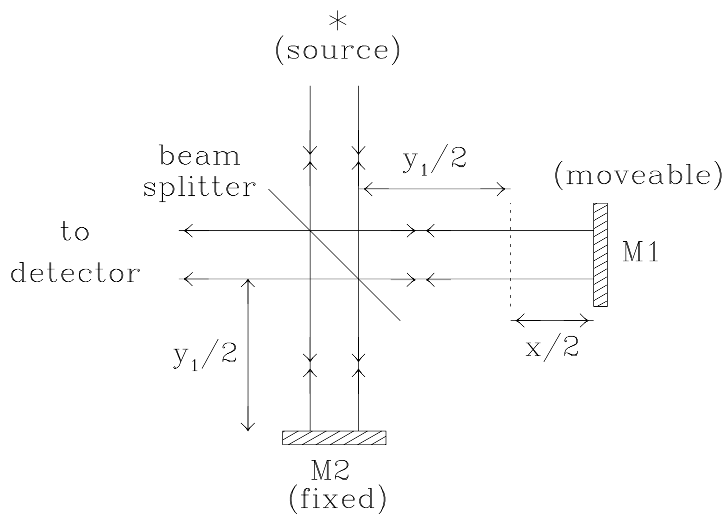

Figure 1: A schematic view of a simple Michelson interferometer. The beam from the source (typically a Hg arc lamp) is collimated and the wavefront is divided at the beam splitter. One arm of the interferometer consists of a fixed mirror, while the other arm contains a moveable mirror. The beams are recombined at the beam splitter after having been reflected once and transmitted once, and then proceed to the sample area and detector.

where x is the path difference. By superimposing (or superposition), the resultant E is given by

$$\vec{E}_R = \vec{E}_1 + \vec{E}_2 = 2rtc\vec{E}_m \cos(\omega t - 2\pi y_1) \cos(\pi \bar{\nu} x). \tag{5}$$

The intensity (I) detected is the time average of E^2. More strictly $\vec{E} \times \vec{H}$ (the Poynting vector), but because $|\vec{E}| \propto |\vec{H}|$ this quantity can be described simply by just $|\vec{E}|$, neglecting some constant of proportionality (which is not important). The intensity may be written as:

$$I \propto 4r^2t^2c^2E_m^2 \cos^2(\omega t - 2\pi y_1 \bar{\nu}) \cos^2(\pi \bar{\nu} x) \tag{6}$$

where the time average of the first cosine term is just 1/2. Thus

$$I \propto 2I(\bar{\nu}) \cos^2(\pi \bar{\nu} x), \tag{7}$$

where $I(\bar{\nu})$ is a constant that depends only upon $\bar{\nu}$. This expression may be simplified to

$$I(x) = I(\bar{\nu})[1 + \cos(2\pi \bar{\nu} x)] \tag{8}$$

where $I(x)$ is the *interferogram* form a monochromatic source. The interferogram for a monochromatic source is shown in Fig. 2.

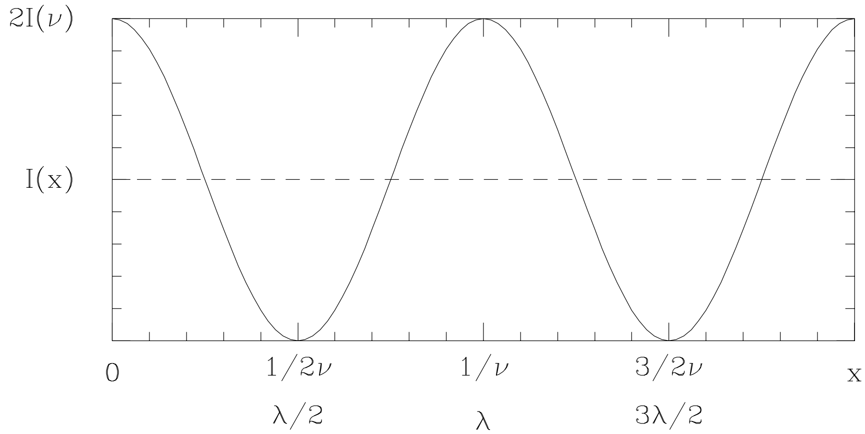

Figure 2: The interference pattern for a monochromatic source (such as a laser) as a function of mirror displacement.

1.1 Polychromatic source

One of the advantages of the Fourier transform instrument is that many different wave numbers may be looked at simultaneously — all the information is gathered at the same time, and we sort it all out using a Fourier transform later. This decreases the measurement time. As well, we can have much more "thruput", i.e. higher intensities and larger solid angles. An interferogram for a polychromatic source which consists of frequencies from $0 \rightarrow \bar{\nu}_m$ is thus:

$$\begin{aligned} I(x) &= \int_0^{\bar{\nu}_m} I(\bar{\nu})[1+\cos(2\pi\bar{\nu}x)]d\bar{\nu} \\ &= \int_0^{\bar{\nu}_m} I(\bar{\nu})d\bar{\nu} + \int_0^{\bar{\nu}_m} I(\bar{\nu})\cos(2\pi x)dx. \end{aligned} \tag{9}$$

When $x = 0$ then

$$\begin{aligned} I(0) &= 2\int_0^{\bar{\nu}_m} I(\bar{\nu})d\bar{\nu} \\ \Rightarrow I(x) &= \frac{1}{2}I(0) + \int_0^{\bar{\nu}_m} I(\bar{\nu})\cos(2\pi\bar{\nu}x)d\bar{\nu}. \end{aligned} \tag{10}$$

With many different wave lengths present, the interferogram resembles the diagram in Fig. 3, which is symmetrical about $x = 0$ for an ideal interferogram.

When $x = 0$ the interference between all of the frequencies is constructive, resulting in a central maxima. However, for $x = \infty$ the frequencies add both constructively and destructively, so that the net contribution due to the

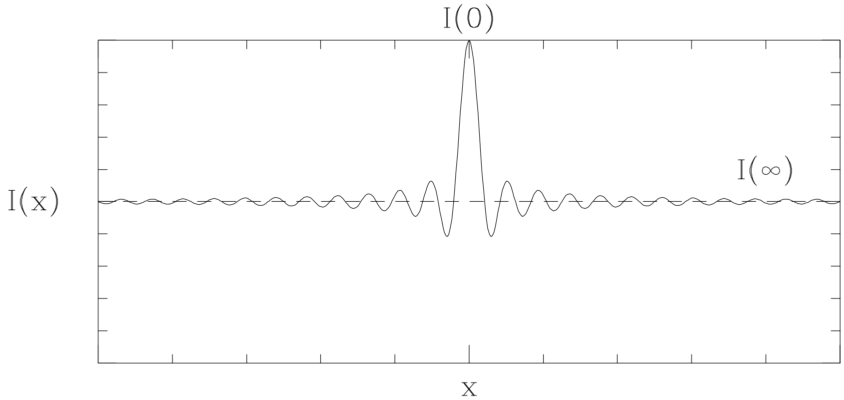

Figure 3: The interference pattern for a polychromatic source about the zero path difference. This curve was generated simply by taking the normalized sum of a number of cosine functions with various frequencies. Note that $I(0) = 2I(\infty)$.

integral in Eq. 10 is simply zero. Thus,

$$I(\infty) = \frac{1}{2} I(0) \tag{11}$$

or more simply, $I(0) = 2I(\infty)$. This relationship is an important check of the instrument alignment.

1.1.1 Percentage modulation

The percentage of modulation is defined as

$$\frac{[I(0) - I(\infty)]}{I(\infty)} \times 100 \tag{12}$$

In a well-aligned instrument, the modulation is $> 85\%$, and this value should be $> 95\%$ in the low frequency region.

1.2 Fourier transform

We have $I(x)$ and now want $I(\bar{\nu})$, i.e.:

$$I(x) - I(\infty) = \int_0^{\bar{\nu}_m} I(\bar{\nu}) \cos(2\pi \bar{\nu} x) d\bar{\nu} \tag{13}$$

letting $\bar{\nu}\_mrightarrow\infty$, we can write

$$I(\bar{\nu}) = \int_0^{\infty} [I(x) - I(\infty)] \cos(2\pi \bar{\nu} x) dx. \tag{14}$$

This procedure involves sampling each position, which can take a long time if the signal is small and the number of frequencies being sampled is large.

1.3 Double-sided interferogram

If $F(x) = I(x) - I(\infty)$, then

$$F(x) = \int_0^{\bar{\nu}_m} I(\bar{\nu}) \cos(2\pi\bar{\nu}x) d\bar{\nu} \tag{15}$$

is symmetric about $x = 0$ since cosine is an even function. However, what if the interferogram behaves differently for $-x$ and $+x$; i.e. you have not sampled at the true zero path difference.

Loss of symmetry can be represented by an additional phase factor:

$$F(x) = \int_0^{\bar{\nu}_m} I(\bar{\nu}) \cos\left[2\pi\bar{\nu}x - \phi\right] d\bar{\nu} \tag{16}$$

$$\begin{aligned} &= \int_0^{\bar{\nu}_m} I(\bar{\nu}) \cos\phi \cos(2\pi\bar{\nu}x) d\bar{\nu} \\ &\quad + \int_0^{\bar{\nu}_m} I(\bar{\nu}) \sin\phi \sin(2\pi\bar{\nu}x) d\bar{\nu}. \end{aligned} \tag{17}$$

What we would like to do is to find a method to be able to deal with the problem of not being at the true zero path difference. For this, we use the complex Fourier transform.

1.3.1 Complex Fourier transform

The complex Fourier transform is defined in the following way:

$$\begin{aligned} g(\bar{\nu}) &= \int_{-\infty}^{\infty} f(x) e^{2\pi i\bar{\nu}x} dx \\ &= \int_{-\infty}^{\infty} f(x) \cos(2\pi\bar{\nu}x) dx + i \int_{-\infty}^{\infty} f(x) \sin(2\pi\bar{\nu}x) dx. \end{aligned} \tag{18}$$

The inverse transform is given by

$$\begin{aligned} f(x) &= \int_{-\infty}^{\infty} g(\bar{\nu}) e^{-2\pi i\bar{\nu}x} d\bar{\nu} \\ &= \int_{-\infty}^{\infty} g(\bar{\nu}) \cos(2\pi\bar{\nu}x) d\bar{\nu} - i \int_{-\infty}^{\infty} g(\bar{\nu}) \sin(2\pi\bar{\nu}x) d\bar{\nu}. \end{aligned} \tag{19}$$

If $f(x)$ is even, $[f(x) = f(-x)]$ then

$$\begin{aligned} g(\bar{\nu}) &= \int_{-\infty}^{\infty} f(x)\cos(2\pi\bar{\nu}x)dx \\ &= 2\int_{0}^{\infty} f(x)\cos(2\pi\bar{\nu}x)dx. \end{aligned} \tag{20}$$

This is referred to as a *cosine transform.* Likewise, if $f(x)$ is odd, then

$$\begin{aligned} g(\bar{\nu}) &= i\int_{-\infty}^{\infty} f(x)\sin(2\pi\bar{\nu}x)dx \\ &= 2i\int_{0}^{\infty} f(x)\sin(2\pi\bar{\nu}x)dx, \end{aligned} \tag{21}$$

is a *sine transform.* Thus, we write

$$g(\bar{\nu}) = C(\bar{\nu}) + iS(\bar{\nu}). \tag{22}$$

Returning to the problem of the interferogram, let $F(x) \equiv f(x)$, [which is $I(x) - I(\infty)$]. then

$$\begin{aligned} C(\bar{\nu}_1) &= \int_{0}^{\bar{\nu}_m} I(\bar{\nu})\cos\phi\left[\int_{-\infty}^{\infty}\cos(2\pi\bar{\nu}x)\cos(2\pi\bar{\nu}_1 x)dx\right]d\bar{\nu} \\ &\quad + \int_{0}^{\bar{\nu}_m} I(\bar{\nu})\sin\phi\left[\int_{-\infty}^{\infty}\sin(2\pi\bar{\nu}x)\sin(2\pi\bar{\nu}_1 x)dx\right]d\bar{\nu}. \end{aligned} \tag{23}$$

Now,

$$\begin{aligned} \int_{-\infty}^{\infty}\cos(2\pi\bar{\nu}x)\cos(2\pi\bar{\nu}_1)x)dx &= \frac{1}{2}\int_{-\infty}^{\infty}\left[e^{2\pi i(\bar{\nu}+\bar{\nu}_1)x} + e^{2\pi i(\bar{\nu}-\bar{\nu}_1)x}\right]dx \\ &= \frac{1}{2}\left[\delta(\bar{\nu}+\bar{\nu}_1) + \delta(\bar{\nu}-\bar{\nu}_1)\right]. \end{aligned} \tag{24}$$

where δ is the Dirac δ function. Note that the sine terms go to zero in the integral when the limits are from $-\infty \to \infty$. This is of the form

$$\delta(\bar{\nu} + L) = \int_{-\infty}^{\infty} e^{2\pi i(\bar{\nu}+L)x}dx \tag{25}$$

In the expression for $C(\bar{\nu}_1)$ we have the product of a sine and a cosine in the interior of the second integral. However, as the sine is a odd function, then its value over the range $-\infty \to \infty$ will be zero. Thus, we can write $C(\bar{\nu}_1)$ as

$$\begin{aligned} C(\bar{\nu}_1) &= \frac{1}{2}\int_0^{\bar{\nu}_m} I(\bar{\nu})\cos\phi\,[\delta(\bar{\nu}+\bar{\nu}_1)+\delta(\bar{\nu}-\bar{\nu}_1)]\,d\bar{\nu} \\ \Rightarrow C(\bar{\nu}_1) &= \frac{I(\bar{\nu}_1}{2}\cos\phi; \quad I(-\bar{\nu}_1)=0. \end{aligned} \tag{26}$$

since $I(\bar{\nu}) = 0$ for all $\bar{\nu} > \bar{\nu}_m$ and for all $\bar{\nu} < 0$. Similarly,

$$S(\bar{\nu}_1) = \frac{I(\bar{\nu}_1)}{2}\sin\phi. \tag{27}$$

Thus

$$\begin{aligned} |g(\bar{\nu}_1)| &= \left[C^2(\bar{\nu}_1)+S^2(\bar{\nu}_1)\right]^{1/2} \\ &= \frac{1}{2}I(\bar{\nu}_1)(\sin^2\phi+\cos^2\phi)^{1/2} \\ &= \frac{I(\bar{\nu}_1)}{2} \end{aligned}$$

so that finally

$$\begin{aligned} I(\bar{\nu}_1) &= 2|g(\bar{\nu}_1)| \\ &= 2\left[C^2(\bar{\nu}_1)+S^2(\bar{\nu}_1)\right]^{1/2} \end{aligned} \tag{28}$$

Thus, the phase error introduced by not sampling symmetrically and the asymmetry in the interferometer is eliminated by taking the the two-sided interferogram and performing a complex fast Fourier transform.

Disadvantages: a factor of two in the data collection time, because the interferogram must be two sided.

1.4 Finite integration limits

In practice the interferogram is from $-x_{max}$ to $+x_{max}$, not $-\infty$ to ∞. To examine the effect, consider the *monochromatic* wave in an ideal interferometer. From Eqs. 6 or 13 (neglecting the constant offset) we get

$$F(x) = I(\bar{\nu}_1)\cos(2\pi\bar{\nu}_1 x) \tag{29}$$

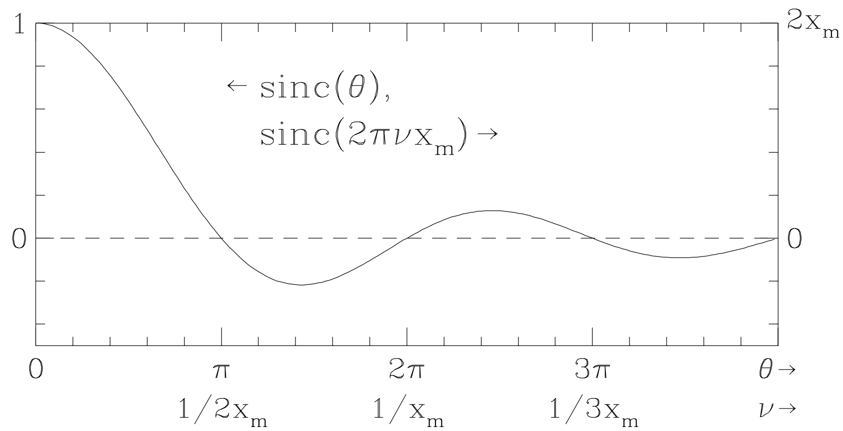

Figure 4: The function sinc(θ) for the rectangular aperture function.

where $F(x)$ is just the structure. We can do the finite transform over the finite range, which may be written as:

$$\int_{-\infty}^{\infty} I(\bar{\nu}_1)\cos(2\pi\bar{\nu}_1 x)e^{2\pi i\bar{\nu}x}\mathrm{rect}(x)dx \tag{30}$$

which is to say that instead of putting limits on the integral, we use the rectangular function defined by:

$$\mathrm{rect}(x) = \begin{cases} 1 & |x| < x_{max} \\ 0 & |x| > x_{max} \end{cases} \tag{31}$$

1.4.1 The convolution theorem

The Fourier transform of the product of two functions, i.e. $f(x)$ and $g(x)$ is the convolution of their individual Fourier transforms $F(y)$ and $G(y)$, where the convolution is defined by

$$F * G = \int_{-\infty}^{\infty} G(u)F(y-u)du \tag{32}$$

The Fourier transform of rect(x) is then

$$\begin{aligned}
\int_{-\infty}^{\infty} \mathrm{rect}(x)e^{2\pi i\bar{\nu}x}dx &= \int_{-x_m}^{x_m} e^{2\pi i\bar{\nu}x}dx \\
&= \int_{-x_m}^{x_m} \left[\cos(2\pi\bar{\nu}x) + i\sin(2\pi\bar{\nu}x)\right]dx \\
&= \left[\frac{\sin(2\pi\bar{\nu}x)}{2\pi\bar{\nu}} - i\frac{\cos(2\pi\bar{\nu}x)}{2\pi\bar{\nu}}\right]_{-x_m}^{x_m}
\end{aligned}$$

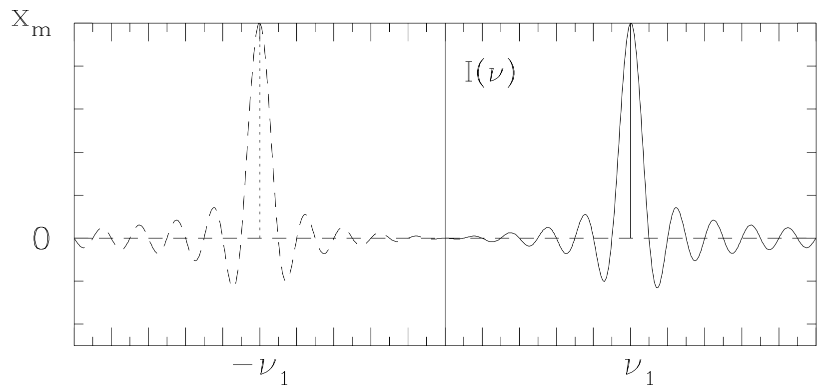

Figure 5: The convolution of the delta function from a single monochromatic source at $\pm\bar{\nu}_1$ and a rectangular aperture function. While the response from the negative side extends into the positive region, it is usually very small and it is ignored. Note that the Fourier transform of the rectangular aperture function is called the instrumental line shape (ILS).

$$
\begin{aligned}
&= \frac{2\sin(2\pi\bar{\nu}x_m)}{2\pi\bar{\nu}} \\
&= 2x_m\frac{\sin(2\pi\bar{\nu}x_m)}{2\pi\bar{\nu}x_m} \\
&= 2x_m\mathrm{sinc}(2\pi\bar{\nu}x_m). \qquad (33)
\end{aligned}
$$

This function is shown in Fig. 4. The Fourier transform of the structure $F(x)$ due to the monochromatic source is:

$$
\begin{aligned}
\int_{-\infty}^{\infty} I(\bar{\nu}_1)\cos(2\pi\bar{\nu}_1 x)e^{2\pi i\bar{\nu}x}dx &= \frac{1}{2}\int_{-\infty}^{\infty} I(\bar{\nu}_1)\left[e^{2\pi i\bar{\nu}x} + e^{-2\pi i\bar{\nu}_1 x}\right]e^{2\pi i\bar{\nu}_1 x}dx \\
&= \frac{1}{2}\int_{-\infty}^{\infty} I(\bar{\nu}_1)\left[e^{2\pi i(\bar{\nu}+\bar{\nu}_1)x} + e^{2\pi i(\bar{\nu}-\bar{\nu}_1)x}\right]dx \\
&= \frac{1}{2}I(\bar{\nu}_1)\left[\delta(\bar{\nu}+\bar{\nu}_1) + \delta(\bar{\nu}-\bar{\nu}_1)\right] \qquad (34)
\end{aligned}
$$

This function is simply two delta functions located at $\pm\bar{\nu}_1$. We usually discard the the negative frequency as it is unphysical, thus we are simply left with the frequency $\bar{\nu}_1$ of the monochromatic source.

The convolution theorem of two transforms is then:

$$
\begin{aligned}
&\int_{-\infty}^{\infty} 2x_m\mathrm{sinc}(2\pi u x_m)\frac{1}{2}I(\bar{\nu})\left[\delta(\bar{\nu}+\bar{\nu}_1+u) + \delta(\bar{\nu}-\bar{\nu}_1+u)\right]du \\
= \ & I(\bar{\nu}_1)x_m\left\{\mathrm{sinc}[2\pi(\bar{\nu}+\bar{\nu}_1)x_m] + \mathrm{sinc}[2\pi(\bar{\nu}-\bar{\nu}_1)x_m]\right\} \qquad (35)
\end{aligned}
$$

which is shown in Figure 5.

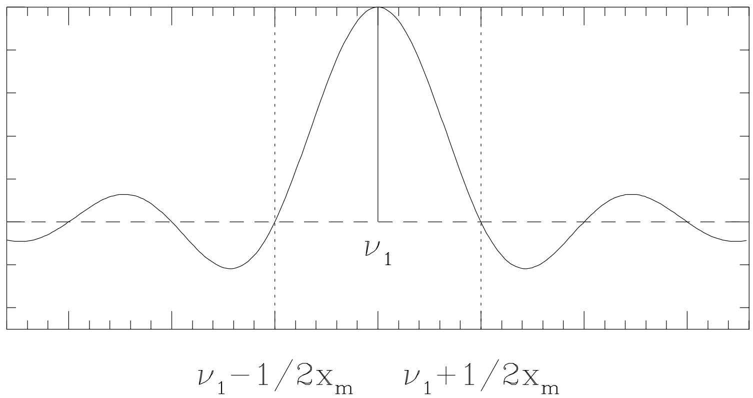

Figure 6: The first two zeros of a sinc function, which occur at $\bar{\nu}_1 \pm 1/2x_m$.

The total from the negative side extends into the positive region, but is usually very small and ignored. Thus:

$$I(\bar{\nu}) = I(\bar{\nu}_1) x_m \mathrm{sinc}[2\pi(\bar{\nu} - \bar{\nu}_1) x_m]. \tag{36}$$

The function $2x_m \mathrm{sinc}(2\pi\bar{\nu}x_m)$ is called the *instrumental line shape* (ILS) or the *spectral window.*

$$I(\bar{\nu}) = I(\bar{\nu}_1) * \mathrm{ILS}. \tag{37}$$

1.4.2 Resolution

Clearly, the ILS has a given width for a monochromatic line. Jacquinot defined the resolution as the distance between the first two zeros on either side of the peak, which is shown in Figure 6 for a sinc function.

Thus,

$$\delta_{\bar{\nu}} = \frac{1}{x_m}. \tag{38}$$

(Note that this delta function is not the Dirac delta function.) Thus, the resolution depends on the length of the scan, i.e. if the mirror scan is 5 cm (which is $x_m/2$), then $x_m = 10$ cm, $\Rightarrow \delta_{\bar{\nu}} = 0.1$ cm^{-1}.

1.5 Apodisation

The "side lobes" or "feet" of the sinc function drop off 22% below zero, which is clearly unacceptable. The problem is in choosing the aperture. The sharp edges produced by the rectangular function introduce this ringing in the spectrum. Thus, what we need is a gentler aperture function. The imposition of such a function is called *apodisation.* The most common apodisation function is the triangular aperture, which is defined as:

$$\mathrm{tri}(x) = \begin{cases} 0 & |x| \geq x_m \\ 1 - |x|/x_m & |x| < x_m \end{cases} \tag{39}$$

However, there are still discontinuities in $\mathrm{tri}(x)$ at $x = 0$ and at $x = \pm x_m$. The Fourier transform of $\mathrm{tri}(x)$ is

$$\begin{aligned} \text{F.T.}[\mathrm{tri}(x)] &= \int_{-\infty}^{\infty} \mathrm{tri}(x) e^{2\pi i \bar{\nu} x} dx \\ &= \int_{-x_m}^{x_m} \left(1 - \frac{|x|}{x_m}\right) e^{2\pi i \bar{\nu} x} dx \\ &= \int_{-x_m}^{x_m} \cos(2\pi\bar{\nu}x) dx + i \int_{-x_m}^{x_m} \sin(2\pi\bar{\nu}x) dx \\ & \quad - \frac{1}{x_m} \int_{-x_m}^{x_m} |x| \cos(2\pi\bar{\nu}x) dx - \frac{i}{x_m} \int_{-x_m}^{x_m} |x| \sin(2\pi\bar{\nu}x) dx \end{aligned} \tag{40}$$

since $\sin(2\pi\bar{\nu}x)$ and $|x|\sin(2\pi\bar{\nu}x)$ are odd functions, then the integrals are identically zero, and thus Eq. 40 reduces to two terms:

$$= \frac{2\sin(2\pi\bar{\nu}x_m)}{2\pi\bar{\nu}} - \frac{2}{x_m} \int_0^{x_m} x \cos(2\pi\bar{\nu}x) dx \tag{41}$$

From a general calculus theorem, recall that

$$\int_a^b f(x) g(x) dx = \left[f(x) \int_0^x g(y) dy \right]_a^b - \int_a^b \frac{\partial f(x)}{\partial x} \left[\int_0^x g(y) dy \right] dx \tag{42}$$

then Eq. 40 becomes

$$\begin{aligned} &= \frac{2\sin(2\pi\bar{\nu}x_m)}{2\pi\bar{\nu}} - \frac{2}{x_m} \left\{ \left[\frac{x \sin(2\pi\bar{\nu}x)}{2\pi\bar{\nu}} \right]_0^{x_m} - \int_0^{x_m} \frac{\sin(2\pi\bar{\nu}x)}{2\pi\bar{\nu}} dx \right\} \\ &= \frac{2\sin(2\pi\bar{\nu}x_m)}{2\pi\bar{\nu}} - \frac{2}{x_m} \left\{ \frac{x_m \sin(2\pi\bar{\nu}x_m)}{2\pi\bar{\nu}} + \left[\frac{\cos(2\pi\bar{\nu}x)}{(2\pi\bar{\nu})^2} \right]_0^{x_m} \right\} \\ &= -\frac{2}{x_m} \left[\frac{\cos(2\pi\bar{\nu}x_m) - 1}{(2\pi\bar{\nu})^2} \right] \\ &= \frac{2}{x_m} \left[\frac{2\sin^2(\pi\bar{\nu}x_m)}{(2\pi\bar{\nu})^2} \right] \\ &= \frac{x_m \sin^2(\pi\bar{\nu}x_m)}{(\pi\bar{\nu}x_m)^2} \\ &= x_m \mathrm{sinc}^2(\pi\bar{\nu}x_m) \end{aligned} \tag{43}$$

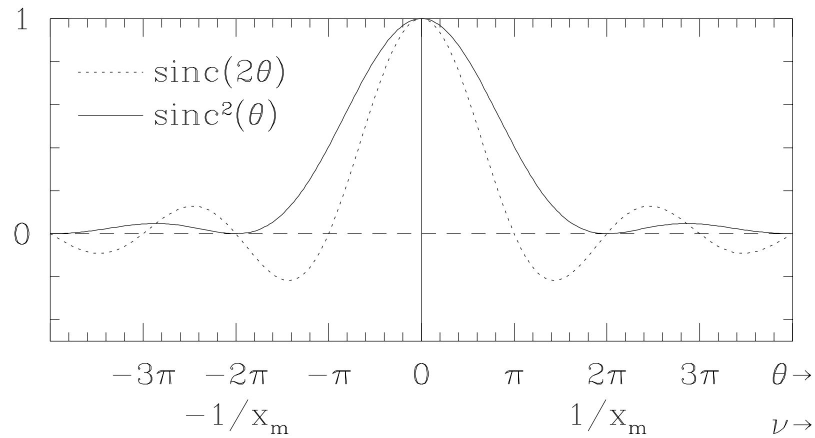

Figure 7: A comparison of the Fourier transforms of the rectangular and triangular aperture functions, sinc(2θ) and sinc$^2(\theta)$ respectively. Note that the Fourier transform of the triangular aperture function has much smaller side lobes, but is broader than the Fourier transform of the rectangular aperture.

The Fourier transform of tri(x) is shown in Fig. 7. Notice the absence of negative side lobes, the small size of the first positive lobes and the increase in the line width. Once again, a monochromatic line $\bar{\nu}$ would give a spectrum given by

$$\begin{aligned} I(\bar{\nu}) &= I(\bar{\nu}_1) * \mathrm{ILS} \\ &= I(\bar{\nu}_1) x_m \mathrm{sinc}^2(\pi \bar{\nu} x_m). \end{aligned} \tag{44}$$

1.5.1 Resolution

If we used the previous definition of resolution, the we would now have

$$\delta_{\bar{\nu}} = \frac{2}{x_m} \tag{45}$$

However, one normally adopts the Rayleigh criterion when attempting to resolve two close lines, which is obtained when when the first zero of one line falls upon the maximum of the other line. When this condition is achieved, the dip between the two lines represents 22% of their maxima. (It should be noted that this assumes that the lines are of equal widths and strengths.) Thus, once again we have that the resolution is given by

$$\delta_{\bar{\nu}} = \frac{1}{x_m}. \tag{46}$$

There are many different kinds of apodisation functions, having a varying

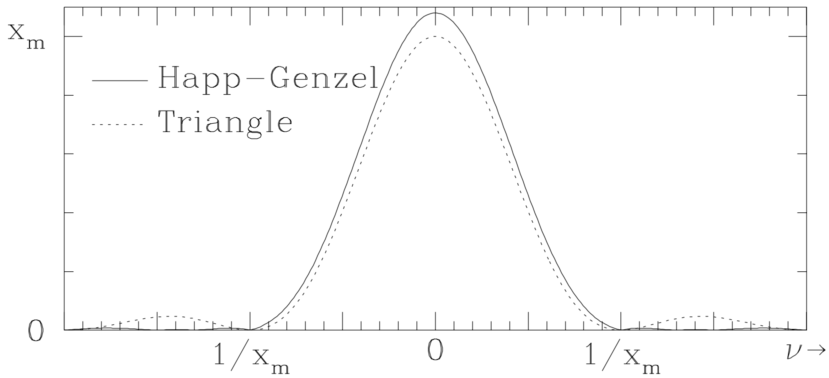

Figure 8: A comparison of the Fourier transforms of the Triangular and Happ-Genzel aperture functions. Note that the side lobes of the Happ-Genzel function are much smaller than those of the triangular apodisation function.

widths and side lobes. A function that has commonly been used is the Happ-Genzel function

$$W(x) = 0.54 + 0.46\cos\left(\frac{\pi x}{x_m}\right). \tag{47}$$

The Fourier transform of the Happ-Genzel function is

$$\text{F.T.}[W(x)] = \frac{sin(2\pi\bar{\nu}x_m)}{2\pi}\left[\frac{1.08}{\bar{\nu}} + \frac{0.46}{x_m/w - \bar{\nu}} - \frac{0.46}{x_m/2 + \bar{\nu}}\right]. \tag{48}$$

A comparison of the Triangular and Happ-Genzel apodisation functions is shown in Figure 8. While the full width at half maximum for the two functions is about the same, the side lobes are almost totally absent in the Happ-Genzel function. In general, we will be using either three or four-term Blackwood-Harris apodisation functions, which have slightly narrower line shapes and very small side lobes.

1.6 Sampling interval

The data has to bee digitized for the Cooley-Tukey fast Fourier transform algorithm in equal increments of path difference Δx. In many early instruments, the data was collected by a "step and integrate" method. Later instruments, such as the Bruker IFS113, adopted a "rapid scan" technique where the infrared radiation is modulated (typically in the kHz frequency range), and many interferograms are taken and averaged. This technique is generally superior to the step-and-integrate method.

The disadvantage of digitizing data in equal increments is the loss of symmetry in the interferogram if the zero-path difference is not sampled and the subsequent inability to detect spurious noise.

1.6.1 The Shah function

The sampled interferogram $F_s(x)$ is related to the complete interferogram $F_c(x) = [I(x) - I(\infty)]_c$ by:

$$F_s(x) = ⫛\left(\frac{x}{\Delta x}\right) F_c(x) \tag{49}$$

where ⫛ (x) is a "combing" function, or Shah function defined by

$$⫛\,(x) = \sum_{-\infty}^{\infty} \delta(x - n) \tag{50}$$

where $\delta(x-n)$ is a Dirac delta function, and n is an integer. Thus, from Eq. 50 the Shah function allows only non-zero value for integers (both positive and negative). Thus, in Eq. 49 the Shah function will allow non-zero value for

$$x = 0, \pm\Delta x, \pm 2\Delta x, \cdots, \pm n\Delta x, \cdots$$

Before proceeding, consider some of the properties of the Shah function. It is periodic (since the limits run from $-\infty$ to ∞)

$$⫛\,(x + m) = ⫛\,(x). \tag{51}$$

We may also derive a scaling rule for the Shah function. Suppose one has

$$⫛\,(ax) = \sum_{n=-\infty}^{\infty} \delta(ax - n) \tag{52}$$

we would like to change the variable from $ax - n$ to $x - n/a$. If we consider the fitting property of the delta function, then

$$\int_{-\infty}^{\infty} \delta\left(x - \frac{n}{a}\right) f(x)dx = f\left(\frac{n}{a}\right) \tag{53}$$

and

$$\begin{aligned} \int_{-\infty}^{\infty} \delta(ax - n) f(x)dx &= \frac{1}{|a|}\int_{-\infty}^{\infty} \delta(y) f\left(\frac{y+n}{a}\right) dy \\ &= \frac{1}{|a|} f\left(\frac{n}{a}\right); y = ax - n. \end{aligned} \tag{54}$$

Comparing Eqs. 53 and 54 one has

$$\delta(ax-n)=\frac{1}{|a|}\delta\left(x-\frac{n}{a}\right) \tag{55}$$

thus

$$⫛\,(ax)=\frac{1}{|a|}\sum_{n=-\infty}^{\infty}\delta\left[x-\left(\frac{n}{a}\right)\right]. \tag{56}$$

We need to know what the effect of the Fourier transform is upon the Shah function.

$$\text{F.T.}[⫛\,(ax)]=\frac{1}{|a|}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\delta\left(x-\frac{n}{a}\right)e^{2\pi i\bar{\nu}x}dx \tag{57}$$

using the sifting property of the δ function gives that

$$\begin{aligned}\text{F.T.}[⫛\,(ax)] &= \frac{1}{|a|}\sum_{n=-\infty}^{\infty}e^{2\pi i\bar{\nu}n/a} &(58)\\ &= \frac{1}{|a|}\left\{\sum_{-\infty}^{\infty}cos\left[2\pi\left(\frac{\bar{\nu}}{a}\right)n\right]+i\sum_{-\infty}^{\infty}sin\left[2\pi\left(\frac{\bar{\nu}}{a}\right)n\right]\right\}. &(59)\end{aligned}$$

In the cosine summation, whenever $\bar{\nu}/a \neq$ an integer value, the cosines will add randomly to zero. However, when $\bar{\nu}=$ an integer, then we get an infinite number of unities adding together. This is the definition of a δ function. Therefore,

$$\text{F.T.}[⫛\,(ax)]=\frac{1}{|a|}\sum_{n=-\infty}^{\infty}\delta\left[\left(\frac{\bar{\nu}}{a}\right)-n\right] \tag{60}$$

and

$$\text{F.T.}[⫛\,(ax)]=\frac{1}{|a|}⫛\left(\frac{\bar{\nu}}{a}\right). \tag{61}$$

The Fourier transform of the Shah function is another Shah function that is reciprocal to the first.

Returning to the spectrum

$$I_s(\bar{\nu})=\text{F.T.}\left[F_s(x)\right] \tag{62}$$

and

$$I_c(\bar{\nu})=\text{F.T.}\left[F_c(x)\right] \tag{63}$$

then

$$
\begin{aligned}
I_s(\bar{\nu}) &= \text{F.T.}\left[⫛ \left(\frac{x}{\Delta x}\right) F_c(x)\right] \quad \text{[from (48)]} && (64)\\
&= \text{F.T.}\left[⫛ \left(\frac{x}{\Delta x}\right)\right] * I_c(\bar{\nu}) && (65)\\
&= \Delta x ⫛ (\bar{\nu}\Delta x) * I_c(\bar{\nu}) \qquad \text{[from (61)]} && (66)\\
&= \Delta x \sum_{n=-\infty}^{\infty} \delta(\bar{\nu}\Delta x - n) * I_c(\bar{\nu}) \quad \text{[from (49)]} && (67)\\
&= \sum_{n=-\infty}^{\infty} \delta\left(\bar{\nu} - \frac{n}{\Delta x}\right) * I_c(\bar{\nu}) \quad \text{[from (55)]} && (68)\\
&= \sum_{n=-\infty}^{\infty} I_c\left(\bar{\nu} - \frac{n}{\Delta x}\right) && (69)
\end{aligned}
$$

so that we finally arrive at

$$I_s(\bar{\nu}) = \sum_{n=-\infty}^{\infty} I_c(\bar{\nu} - n\Delta\bar{\nu}) \tag{70}$$

where

$$\Delta\bar{\nu} = \frac{1}{\Delta x}. \tag{71}$$

Thus, when transforming the sampled interferogram, we get an infinite number of complete spectra, each starting at $n\Delta\bar{\nu}$. The transformed spectra are actually the sum of the spectra for the positive frequencies and those of the negative frequencies from an adjacent spectra. Incorrect choices of a sampling frequency can lead to large contributions to distortions of the spectra. This is called “aliasing” or “false energies”. In order to avoid this, one must make $\Delta\bar{\nu}$ large enough so that the maximum frequency contribution of the positive $\bar{\nu}$ spectrum does not overlap with the negative $\bar{\nu}$ spectrum. This may be accomplished by requiring that

$$\Delta\bar{\nu} \geq 2\bar{\nu}_{max} \tag{72}$$

or

$$\Delta x \leq \frac{1}{2\bar{\nu}_{max}}. \tag{73}$$

In term of wave number regions, this results in the following conditions: Another way of seeing the condition that $\Delta x \leq 1/2\bar{\nu}_{max}$ is that $\Delta x \leq \lambda_{min}/2$,

Table 1: The minimum sampling interval required to prevent aliasing for the wave number range from $0 \to \bar{\nu}_{max}$.

$\bar{\nu}_{max}$ (cm^{-1})	Δx (μm)
2000	2.5
1000	5
500	10
250	20
125	40
62.5	80

which means that one must sample at least every twice in every cycle of the smallest wave length of radiation in the interferogram (this is just the Nyquist frequency from information theory).

Having chosen $\bar{\nu}_{max}$, and found the appropriate Δx, one must make certain that there is no radiation with $\bar{\nu} > \bar{\nu}_{max}$ by the use of optical filters.